TOXIC SUBSTANCES CONTROL ACT INVENTORY REPRESENTATION FOR

POLYMERIC SUBSTANCES

I. Introduction

This paper explains the conventions that are applied to listings of polymeric chemical substances for the Chemical Substance Inventory that is maintained by the U.S. Environmental Protection Agency (EPA) under the Toxic Substances Control Act (TSCA). These conventions have been in place largely without changes since the inception of the Inventory. The Agency's goal in developing this paper is to make it easier for the users of the Inventory to interpret listings for polymers and to understand how new substances should be identified for Inventory inclusion.

Fundamental to the Inventory as a whole is the principle that entries on the Inventory are identified as precisely as possible for the commercial chemical substance, as reported by the submitter. Substances that are chemically indistinguishable, or even identical, may be listed differently on the Inventory, depending on the degree of knowledge that the submitters possess and report about such substances, as well as how submitters intend to represent the chemical identities to the Agency and to customers. Although these chemically indistinguishable substances are named differently on the Inventory, this is not a "nomenclature" issue, but an issue of substance representation. Submitters should be aware that their choice for substance representation plays an important role in the Agency's determination of how the substance will be listed on the Inventory.

A. Polymer Definition

For the purposes of the TSCA Inventory, a substance must meet the following compositional requirements in order to be considered a polymer:

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1) The molecules are characterized by a sequence of one or more types of monomer units (where a monomer unit is the reacted form of the monomer in a polymer bonded to two or more other molecules);

2) There is a molecular weight distribution among the molecules present in the chemical substance that is primarily attributable to differences in the number of monomer units contained in the molecules.

An Inventory listing for each polymer describes a category

of possible chemicals that would fit that substance name, instead of just representing a single molecular structure. The molecules that fall within a given Inventory listing for a polymer vary in molecular weight; they may also vary in composition (i.e., in the ratios of the starting monomers and other reactants used in the polymer) so long as every monomer or other reactant mentioned in the name is, in fact, part of each polymer molecule, either as a whole molecule or a fragment. Polymers may also contain small amounts of other monomers and reactants that are not part of the name; the conventions applicable to this area are stated in section II.D.1., The Two Percent Rule, below. The Agency's approach to polymer nomenclature gives manufacturers and importers considerable flexibility to make minor changes in their products without the requirement of a Premanufacture Notification (PMN).

B. Certain Resinous Substances are not Polymers

Some industry segments have traditionally regarded certain resinous substances as polymers, such as the glycerol or pentaerythritol esters of rosin. The Agency believes that such resinous substances are simple esters of rosin (a monobasic acid), which consist of various adducts (alcohol:acid molecular ratios of 1:1, 1:2, 1:3, etc.), depending on the ratio of polyhydric alcohols and rosin used. There are neither sequences of monomer units in the structures nor molecular weight distributions attributable to various degrees of polymerization of monomers and other reactants. These types of substances are usually described for TSCA purposes with non-polymer names that include the term "ester with" or "esters with... ."

II. Inventory Representation with Examples

A. Introduction to Monomer-based versus Structural Repeating Unit Nomenclature

Polymeric substances are represented on the TSCA Inventory in one of two ways. Depending on the type of polymer, either a monomer-based representation or a structural repeating unit representation (SRU) will be used. In either case, the Agency generally attempts to name chemical substances as specifically as possible, based on the chemical structure information known by the submitter.

1. Monomer-based Representation

Most polymers (with the exception of certain polyglycols and derivatives, and siloxanes and silicones) are represented on the Inventory in terms of the starting materials from which they are manufactured. In fact, more than 80% of the polymers on the TSCA Inventory are listed in terms of starting materials. This so-called monomer-based representation is used when a polymeric substance cannot be identified by a single definite structural diagram and when either of the following conditions is met:

1) when the polymer contains only one constituent monomer and the degree of polymerization is unknown or the polymer is reported in terms of molecular weight distribution, or

Exception: Homopolymeric substances with more than ten constituent monomers are named as polymers, even if

they have definite structural diagrams.

2) when a polymer contains more than one type of constituent monomer in no particular sequence, regardless of the degree of polymerization.

Polymers that use monomer-based representation are described according to the starting monomers used in their manufacture as well as other reactants including free-radical initiators, cross-linking agents, chain transfer agents, mono-functional groups that act as modifiers and other end groups that become chemically incorporated into the polymer structure, subject to the two percent rule (see section II.D.1. for details). The basic form of a typical monomer-based polymer name is Reactant A, polymer with reactant B and reactant C. Examples of simple monomer-based polymers are:

Example 1. Formaldehyde, polymer with 2-propanone
CASRN 25619-09-4

Example 2. 2-Propenoic acid, polymer with 2,2'-azobis[2-methylpropanenitrile] and butyl 2-propenoate
CASRN 68083-62-5

In this example, the 2,2'-azobis[2-methylpropanenitrile] is a free-radical initiator.

2. Structural Repeating Unit (SRU) Representation

For TSCA purposes, SRU names are only used for several types of common polymer backbones in which the structure of the polymer is known or reasonably ascertained to consist of repeating units instead of being random, and where there is a reported average number of SRU's, a variable range of SRU's, or an unknown number of SRU's. Polymers named with SRU names on the Inventory include certain polyethylene glycols and derivatives, certain polypropylene glycols and derivatives, and siloxanes and silicones.

If these polymers were named strictly according to their constituent reactants or monomers, important structural features of the polymers would not be obvious from the name, and polymers with significantly different properties and applications would have the same name and CASRN. Thus, the use of structural repeating subunit nomenclature more effectively distinguishes polymer products than does the starting monomer approach.

For a given polymeric substance represented by an SRU, the repeating part of the molecular formula is enclosed in parentheses with a subscript "n." The "n" value in the molecular formula can represent either 1) an unknown value, 2) a variable range, 3) an average value, or 4) a specific integral value of at least 11. There is no lower or upper limit to the average number or range of "n" in order to apply SRU nomenclature. An example of a simple SRU polymer is:

Example 3. Poly(oxy-1,4-butanediyl), à-hydro- -hydroxy-
CASRN 25190-06-1
(C4H8O)nH2O

In this example, the value of "n" in the molecular

formula is not defined, but is assumed to meet one of the four criteria above. If "n" were an integral value of less than 11, the substance would be named as a Class 1, discrete substance and not as a polymer.

3. Advantages and Limitations of Monomer-based and SRU Nomenclature

The main advantages associated with polymers named with monomer-based representation are (1) elimination of the need to determine the structure of a polymer in order to report and (2) great flexibility in reactant stoichiometry and polymer molecular weight. Each Inventory listing of this type allows each reactant to be charged at any percentage, and each polymer name covers virtually any molecular weight range. The polymers may vary considerably in structure and properties, while still utilizing the same Inventory name. Thus, each polymer name is considered to describe a category of polymers.

Manufacture according to monomer-based polymer listings has the limitation that only the one specified set of monomers and reactants can be used. Even if a chemically-identical polymer can be formed by different sets of reactants, additional Inventory listings are needed to cover manufacture using other sets of reactants.

In contrast, SRU-based representation has the advantage that manufacturers may substitute starting materials as long as they make the same final product. SRU-based polymer listings have the limitation that the specified structural component must be formed; if the same reactants could, in theory, be used to form a different type of structure, that second structure would require a different Inventory listing.

B. Representation of Specific Monomer-based Polymers

For Inventory representation, specific monomer-based polymers are divided into two classes: homopolymers and copolymers. Each of these is discussed below.

1. Homopolymers

Homopolymers are made from a single monomer and are named according to that monomer identity, with the term "homopolymer" used as a modifier at the end of the name. The chemical formulas of homopolymers are found in the Formula Index of the printed Inventory and in the corresponding fields of computerized database versions of the Inventory.

If the degree of polymerization can be represented by a molecular weight distribution, where the number of monomer units can be expressed by a range or an average value, homopolymer nomenclature is used. For example, the name Propene, homopolymer could represent the following types of molecular formula: (CH3-CH=CH2)5-10 or (CH3-CH=CH2)5.7.

If a polymer based on one monomer contains more than ten monomer units it is named as a homopolymer regardless of whether the degree of polymerization above ten represents a single value, a range, an average value or is unknown. Thus, "Propene, homopolymer" could also represent any of the formulas: (CH3CH=CH2)12, (CH3CH=CH2)14-18, or (CH3CH=CH2)n>10. This definition of the term homopolymer is the sole exception to the TSCA

requirement that a molecular weight distribution exist in order to consider a substance a polymer. For example, (CH3CH=CH2)12 has no molecular weight distribution, yet is named as a polymer.

If the degree of polymerization of a substance is a single, integral value of ten (10) or fewer, the substance is not a polymer and is named as a Class 1 substance. For example, a propene "homopolymer" with the degree of polymerization n=4 and a structure (CH3CH=CH2)4 would be named 1-Propene, tetramer (CASRN 6842-15-5).

2. Copolymers

Copolymers are made from more than one kind of monomer. Typical names for copolymers begin with the name of one monomer, then the term, "polymer with," followed by the other monomers listed in alphabetical order. In general, the most highly functionalized monomer is chosen as the first monomer in the name and the rest of the monomers and other reactants are listed in alphabetical order, based on their CA names. The formula of each monomer that is part of the polymer formula representation is found in the Formula Index of the printed Inventory and in many on-line databases of Inventory information. Using a molecular formula can simplify finding a specific polymer if one is not sure which monomer would be cited first in the polymer name.

Example 4. 2-Propenoic acid, polymer with ethyl 2-propenoate
CASRN 25085-35-2
(C5H8O2.C3H4O2)x

This is the copolymer of acrylic acid and ethyl acrylate.

In most cases, the phrase "polymer with" is used in the name for a copolymer; if, however, reactant A is plural, the plural phrase "polymers with" is used. See the following examples:

Example 5. Linseed oil, polymer with glycerol and phthalic anhydride
CASRN 66070-59-5*

Example 6. Fatty acids, linseed-oil, polymers with glycerol and phthalic anhydride
CASRN 68309-01-3*

3. Polymers Made from Monofunctional Reactants

If a monofunctional reactant is part of a polymer, the polymer is named so that it is clear that the monofunctional reactant is not part of the polymer backbone, but is appended to it.

Example 7. 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-, polymer with 5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane, caprolactam-blocked
CASRN 68610-70-8*
(C12H18N2O2 . C6H14O3 . C6H11NO)X

Example 8. 1,3-Butadiene, homopolymer, hydroxy-terminated
CASRN 69102-90-5*

Exception: Polymers involving fats and oils and their fatty

acids are named with all components being treated equally as monomers, even though some may be monofunctional and could be considered to be modifying agents.

Example 9. Tall oil, polymer with benzoic acid, ethylene glycol, glycerol, pentaerythritol and phthalic anhydride
CASRN 68477-14-5*

In this case, both tall oil and benzoic acid are monofunctional reactants.

4. Post-Treated Polymers

Certain modifying or derivative information, such as indicated by the auxiliary terms blocked, terminated, oxidized, ether, ester, etc., will also appear in the polymer name. As a result of this convention, a polymer of A, B and C that is post-treated with D will usually have a different name for TSCA purposes than an ordinary copolymer of A, B, C and D.

Example 10. 1,3-Butadiene, homopolymer, oxidized
CASRN: 68441-53-2*

Example 11. 1,3-Butanediol, polymer with 1,3-diisocyanatomethylbenzene and à-hydro- -hydroxypoly(oxy-1,4-butanediyl), Me Et ketone oxime-blocked
CASRN: 65733-70-2*

Example 12. Phenol, polymer with formaldehyde, glycidyl ether
CASRN 28064-14-4*

This substance (CASRN 28064-14-4*) is a post-treated phenol-formaldehyde polymer which specifically contains pendant glycidyl ether groups. Although this ether group is identified in the substance, the polymer name does not specify whether epichlorohydrin is the actual chemical source of the glycidyl ether moiety, and the degree of incorporation of glycidyl ether groups is not specified.

On the other hand, the random polymer description associated with CASRN 9003-36-5, below, assumes that epichlorohydrin [i.e., (chloromethyl)oxirane] is used as either a reactant or a monomer that is incorporated

in whole or in part somewhere in the polymer structure.

Formaldehyde, polymer with (chloromethyl)oxirane and phenol
CASRN 9003-36-5

The two polymers in this example are considered to be two different substances, even though they could be

manufactured using the same set of monomers and reactants.

5. Copolymers of Rosin, Maleic Anhydride or Fumaric Acid

Copolymers of rosin and maleic anhydride and/or fumaric acid that contain no other oil or oil derivative are named using the term(s) "maleated" and/or "fumarated" as part of the modifying information. Maleic anhydride is assumed to be the "maleating" agent unless maleic acid is specified.

Example 13. Rosin, fumarated maleated, polymer with glycerol
CASRN 68153-44-6*

Example 14. Rosin, maleated, polymer with p-tert-butylphenol, formaldehyde and pentaerythritol
CASRN 68082-96-2*

The terms "maleated" and/or "fumarated" are not used in any other copolymer situation involving rosin. For example, if maleic anhydride or fumaric acid react elsewhere in the polymer besides maleating/fumarating the rosin, the maleic anhydride or fumaric acid would be named as a regular monomer instead of as a modifier, regardless of whether another oil or oil derivative is used.

Example 15. Linseed oil, polymer with fumaric acid and glycerol
CASRN 68514-51-2*

6. Ultimate Monomer Policy (as applied to Pre-neutralized vs. Post-neutralized Polymers)

According to 40 CFR 710.5(c), polymers are typically identified by listing the monomers and other reactants from which they are manufactured. This convention of naming polymers in terms of the starting materials represents a long-standing and widely-accepted agreement between the Agency, industry and Chemical Abstracts Service (CAS). In addition to applying to polymers made directly from monomers, this principle of nomenclature is applicable to naming a polymer made by reacting an existing polymer intermediate or prepolymer with additional monomers/reactants. The name of such a polymer would usually include the monomers from which the existing polymer is made along with the names of other monomers/reactants used. This practice is known as the "Ultimate Monomer Policy."

The following examples illustrate how to apply the "ultimate monomer policy" to certain neutralized polymers manufactured by different processes.

Example 16. When sodium hydroxide is added to a mixture of acrylic acid and acrylamide in the reaction vessel used for polymerization, the ultimate monomers and reactants are considered to be acrylic acid, acrylamide and sodium hydroxide. The resulting polymer would be described as "2-Propenoic acid, polymer with 2-propenamide, sodium salt," CASRN 25987-30-8. If this polymer were then neutralized further with sodium hydroxide, the name would not change.

Example 17. If the manufacturer uses an acrylic acid monomer that has already been partially neutralized with sodium hydroxide by its supplier and polymerizes this acrylic acid/sodium acrylate combination with acrylamide, the "ultimate monomers" are sodium acrylate, acrylic acid and acrylamide. The polymer would be described as "2-Propenoic acid, polymer with 2-propenamide and sodium 2-propenoate," CASRN 62649-23-4. However, if a fully neutralized "sodium acrylate" is charged to the reactor and then polymerizes with acrylamide, the polymer would be described as "2-Propenoic acid, sodium salt, polymer with 2-propenamide," CASRN 25085-02-3.

Example 18. In contrast to Example 16, when a mixture of acrylic acid, sodium acrylate and acrylamide is polymerized and then further neutralized with sodium hydroxide, the resulting polymer would be described as "2-Propenoic acid, polymer with 2-propenamide and sodium 2-propenoate, sodium salt," no CASRN assigned.

Example 19. If acrylamide is added to a reaction vessel containing acrylic acid that was already partially or fully neutralized in the reaction vessel with sodium hydroxide (forming sodium acrylate in situ without isolation), the ultimate monomers/reactants are acrylamide, acrylic acid and sodium hydroxide. The polymer would be named as "2-Propenoic acid, polymer with 2-propenamide, sodium salt," CASRN 25987-30-8, which is the same name as in the Example 16, above.

Example 20. When acrylic acid is partially neutralized with sodium hydroxide, then isolated, followed by polymerization with acrylamide, the ultimate monomers are sodium acrylate, acrylic acid and acrylamide. The resultant polymer name, "2-Propenoic acid, polymer with 2-propenamide and sodium 2-propenoate," CASRN 62649-23-4, is the same as in Example 17.

Whether the monomer is neutralized prior to being added to the polymerization vessel or is neutralized in the polymerization vessel before polymerization is started will affect the naming of the polymer, since the substances actually charged to the reaction vessel are what determine the polymer description.

C. Representation of Structural Repeating Unit Polymers

1. Polyglycols

The name for a polyglycol representable via SRU nomenclature on the Inventory begins with the term "poly," followed by a divalent radical enclosed in parentheses or brackets. The chain

of a polyglycol has terminating groups which are named as modifiers of the base polymer, and given the locants "à" and " ."

Example 21. Poly(oxy-1,2-ethanediyl), à-methyl- -hydroxy-
CASRN 9004-74-4
(C2H4O)nCH4O

The "CH4O" part of the formula corresponds to the sum of the atoms comprising the methyl and hydroxy end groups. This SRU name is appropriate for a polyethylene glycol derivative as long as only water or ethylene glycol(s) is used as the initiator in its manufacture. Such a name does not specify any particular value or range for "n."

Polyethylene glycols and polypropylene glycols are typically manufactured from the corresponding alkylene oxide and an initiator such as water or simple alkyl glycols or polyols. For TSCA purposes, water-initiated and ethylene glycol-initiated polyethylene glycols are considered equivalent.

Example 22. Poly(oxy-1,2-ethanediyl), à-hydro- -hydroxy-
CASRN 25322-68-3

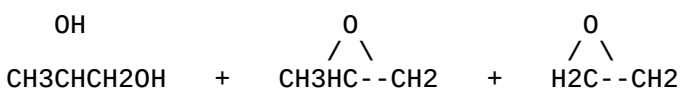
Similarly, water-initiated and propylene glycol-initiated polypropylene glycols are considered equivalent.

Example 23. Poly[oxy(methyl-1,2-ethanediyl)], à-hydro- -hydroxy-
CASRN 25322-69-4

Consequently, for the purposes of TSCA, identical polymers are manufactured when either water-initiated or ethylene glycol-initiated polyethylene glycol is used as a reactant along with the same set of other monomers and reactants. Likewise, other polymers based on either water-initiated or propylene glycol-initiated polypropylene glycol would be identical when the other monomers and reactants are the same.

Polyalkylene glycols are identified in terms of structural repeating units if they are produced by the water-initiated polymerization of ethylene oxide or propylene oxide, the ethylene glycol-initiated polymerization of ethylene oxide, or the propylene glycol-initiated polymerization of propylene oxide. Other polyalkylene glycols or those made from other initiator/alkylene oxide reactants usually require monomer-based nomenclature, as shown below.

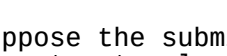
Example 24. 1,2-Propanediol, polymer with methyloxirane and oxirane
CASRN 65395-10-0



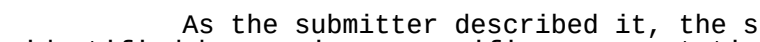
monomer-based name: 1,2-Propanediol, polymer with methyloxirane and oxirane

In determining how an SRU-based substance should be represented on the TSCA Inventory, the submitter's intent as well as the way the chemical is reported are taken into consideration. Thus, if "n" (the number of repeating units) is reported as a single integer whose value is less than 11, the substance has a specific chemical structure and molecular formula and is given a Class 1 name.

Example 25. Consider a substance having the following general formula:



Suppose the submitter specifies that the substance contains four structural repeating units (n=4) with the following structure:



As the submitter described it, the substance is identified by a unique, specific representation (a Class 1 substance name) instead of being named as a polymer. The CA Index name is:

2,5,8,11-Tetraoxatridecan-13-ol
CASRN: 23783-42-8

In the case of mono or unspecified esters or ethers of polyethylene glycol (PEG), polypropylene glycol (PPG) or polyethylene-polypropylene glycol, the terms "ethoxylated" and/or "propoxylated" are used in the modifying information. In all other cases the phrases "ester(s) with," "monoester(s) with,"

"diesters with," or "ether(s) with" are used. SRU's of PEG or PPG involving Class 1 end groups are an exception: the ether or ester end groups are indicated by "à-" and " -" terms that are specifically structural in nature, as shown in Examples 28 and 29.

Example 26. Fatty acids, tall-oil, ethoxylated
CASRN 61791-00-2*

Example 27. Fatty acids, tall-oil, monoesters with polyglycerol
CASRN 61790-95-2*

Example 28. Poly(oxy-1,2-ethanediyl), à-butyl- -hydroxy-
CASRN 9004-77-7
Bu-[OCH2CH2]n-OH

Example 29. Poly(oxy-1,2-ethanediyl), à-acetyl- -(acetyloxy)-
CASRN 27252-83-1

```
   O          O

CH3C-[OCH2CH2]n-OCCH3
```

2. Silicone Polymers

a. General

For the TSCA Inventory, silicone polymers are generally named in terms of structure-based polymer names. Silicone polymers containing the same repeating subunits (and the same terminating groups) can be manufactured from different monomers or combinations of monomers and be covered under the same SRU name for TSCA purposes.

In the representation of silicone polymers, it is always assumed that the polymer is terminated with trimethylsilyl (TMS) groups unless other terminating groups are specified. Consequently, the terminating group, TMS, does not appear in the name.

Example 30. Siloxanes and Silicones, di-Me
CASRN 63148-62-9*

```
        Me   Me    Me
        |    |     |
    Me-SiO-(SiO)n-Si-Me
        |    |     |
        Me   Me    Me
```

If specified, the other (non-TMS) terminating group(s) will be named.

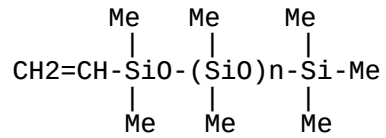
Example 31. Siloxanes and Silicones, di-Me, vinyl group-terminated
CASRN 68083-19-2*

```
        Me   Me    Me
        |    |     |
 CH2=CH-SiO-(SiO)n-Si-CH=CH2
        |    |     |
```

```
                    Me   Me    Me
```

It is always assumed that both ends of the polymer are terminated, either by TMS or by a specified end group(s). If only one end is terminated with a vinyl group, the product will be described as "mono(vinyl group)-terminated," and the other end group is assumed to be terminated with the trimethylsilyl group, which is not included in the name.

Example 32. Siloxanes and Silicones, di-Me, mono(vinyl group)-terminated
CASRN 68952-00-1*



Exception 1: A monomer-based representation is used for silicone polymers when the overall structure for the final product is unknown.

Example 33. Cyclotetrasiloxane, octamethyl-, polymer with 2,4,6,8-tetramethyl-2,4,6,8-tetraphenyl cyclotetrasiloxane
CASRN 68072-44-6

Exception 2: In some cases, the silicone polymer backbone is modified (or terminated) by forming reaction products with another reactant. In such cases, insufficient information is known or given to identify the product completely, and an SRU representation cannot be developed.

Example 34. Siloxanes and Silicones, di-Me, reaction products with Me hydrogen siloxanes and 1,1,3,3-tetramethyldisiloxane
CASRN 69430-47-3*

b. Siloxanes and Silicones

This class is represented by the structural formula (R2SiO)n where R is an alkyl or aryl group. If "n" is a single integer whose value is 2-10, then this substance has a specific substance representation and is given a Class 1 name. If (1) "n" is greater than 10, (2) "n" represents the average number or range of repeating units, or (3) the value of "n" is unknown, the substance is given a polymer name of the SRU type.

Siloxane and silicone polymers are named "Siloxanes and Silicones" and may be modified by two types of substituents: 1) those groups (R-) attached to the silicon atoms in the repeating group and 2) those groups (A-) attached to the oxygen atom as the terminating group.

Example 35. Generically: Siloxanes and Silicones, di-R, A-terminated

```
                    R
```

```
                    |
          A-O-(SiO-)n-A
                    |
                    R
```

The structural representation of silicone polymers is drawn to reveal the structural repeating unit with its substituents and to identify the terminating groups that delineate the SRU. The name given to the polymer describes the product completely.

Example 36. Siloxanes and silicones, Me Ph, hydroxy-terminated
CASRN 80801-30-5*

```
                 Me
                 |
            HO-(SiO-)n-H
                 |
                 Ph
```

Example 37. Siloxanes and silicones, Me Ph
CASRN 63148-58-3*

```
                Me   Me    Me
                |    |     |
          Me-SiO-(SiO)n-Si-Me
                |    |     |
                Me   Ph    Me
```

Example 38. Siloxanes and silicones, di-Me, Me vinyl, mono(vinyl group)-terminated
CASRN 68951-99-5*

```
                Me   Me     Me     Me
                |    |      |      |
      Me-SiO-(SiO)n-(SiO)m---SiCH=CH2
                |    |      |      |
                Me   Me     CH=CH2 Me
```

c. Silsesquioxanes

These polymers are made from trifunctional silanes and are typically large, highly cross-linked molecules. The term silsesquioxanes denotes a polymer in which each silicon atom in the SRU has three atoms attached to it that are shared with other silicone atoms. The ratio of silicon and oxygen in the SRU is 1 to 1.5 (sesqui). Silsesquioxanes may be modified by two types of substituents: those (1) attached to the silicon atom in the repeating group (R- substituents) and (2) the terminating groups (A- substituents).

Example 39. Generically: Silsesquioxanes, R, A-terminated

```
                      R
                      |
            A-(SiO3/2)n-A
```

Example 40. Silsesquioxanes, Ph
CASRN 70131-69-0*

```
                Me   Ph      Me
                |    |       |
          Me-SiO-(SiO3/2)n-Si-Me
```

```
        |          |
       Me         Me
```

d. Cyclosiloxanes

This term denotes silicon-containing chemical substances in which the repeating groups are in a cyclic structure with the ring size unknown. Since these molecules have no terminal end groups, the cyclosiloxanes name may only be modified by the substituent(s), R, attached to the silicon atom in the repeating group. If the repeating unit "n" in a cyclosiloxane is known, it is considered to be a Class 1 substance and is given a specific name. If the ring size is unknown, the substance is named as an unspecified cyclosiloxane.

Example 41.

Cyclosiloxanes, di-Me CASRN 69430-24-6	Cyclotrisiloxane hexamethyl-, CASRN 541-05-9

e. Silicic Acid Polymers

These polymers are made from tetrafunctional silanes such as tetrachlorosilane or tetraalkoxysilane. Silicic acid (CASRN 1343-98-2, which shows no molecular formula with the name) contains silanes and siloxanes in which all hydrogen atoms have been replaced by hydroxyl and oxo groups; it is considered a polymeric substance of unspecified structure. Thus, a silicic acid polymer made from tetraethyl silicic acid will be named simply "Silicic acid, ethyl ester." The term "homopolymer" is not part of the name because it is understood from the name silicic acid that the substance is polymeric.

Example 42.

Silicic acid, ethyl ester CASRN 11099-06-2	Silicic acid (H_4SiO_4) tetraethyl ester CASRN 78-10-4

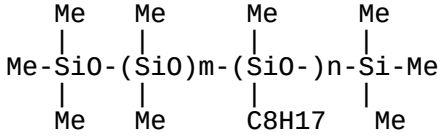
```
          OC2H5
           |
H5C2O-Si-OC2H5
           |
          OC2H5
```

f. Post-Treated Silicone Polymers

Post-treated silicone polymers are named as chemical derivatives of an SRU type name; the name indicates the resultant

structure, as incorporated, of the post-treating reactant.

Example 43. Siloxanes and Silicones, di-Me, Me octyl
CASRN 70900-22-0*



If one did not know the exact structure generated from such a reaction, for example, an alkylation of dimethyl, methyl hydrogen siloxane with 1-octene, a less specific name such as "Siloxanes and Silicones, di-Me, Me hydrogen, alkylation products with 1-octene," CASRN 72623-91-7*, would be used.

D. General Nomenclature Rules

The following rules apply to both monomer-based and SRU polymers.

1. The Two Percent Rule

a. General Statement of the Rule

The description of a polymer must include those monomers and other reactants used at greater than two weight percent (based on the dry weight of the polymer manufactured), where the weight percent of all monomers/reactants used is based either on (A) the weight of reactant charged to the reaction vessel, or (B) the minimum theoretical weight of reactant that would be needed to account for the observed weight of chemically combined (incorporated) reactant molecules or fragments in the polymer [40 CFR 720.45(a)(2)(iv)].

Other additives, such as plasticizers, colorants, UV absorbers, etc., which do not chemically become a part of the polymeric structure are not identified in the description of the polymer. Monomers and other reactants used at two percent or less may be included in the description of the polymer if the submitting company desires, but the submitter must indicate such an intention. Although a submitter may choose to include monomers or other reactive ingredients used at two percent or less for purposes of describing a polymer, he or she is not required to do so under TSCA. Information on these minor monomers/reactants must, however, be reported in the PMN for a polymer. See 40 CFR 720.45(a) for details.

In interpreting a particular polymer listing on the Inventory that does not contain a certain minor monomer or reactant identity, a manufacturer may use either the "charged" method or the "incorporated" method as long as it can be demonstrated that 2% or less of that minor monomer or other reactant is used in the manufacture of its substance, when not intended to be part of the polymer identity.

b. Application of the Two Percent Rule to Free-Radical Initiators

Free-radical initiators used at greater than two weight

percent in the manufacture of a polymer must be included in the description of a polymer for the purposes of Premanufacture Notification and listing on the TSCA Inventory. If the initiator is used at less than or equal to two weight percent the submitter may include the initiator as part of the Inventory listing if he or she wishes.

Example 44. 2-Propenoic acid, 2-methyl-, octadecyl ester, polymer with butyl 2-propenoate and ethenylbenzene, tert-Bu peroxide-initiated
CASRN 118578-04-4*
(C22H42O2.C8H18O2.C8H8.C7H12O2)x

EPA applies this convention only to those polymers not listed on the Inventory as of July 28, 1989, the effective date of the Federal Register Notice that clarified the Agency's interpretation of this rule. All polymer substances that were included on the Inventory as of July 28, 1989 that do not contain the identity of any free-radical initiators in their Inventory names are considered by EPA to cover that polymer manufactured using any free-radical initiator in any amount.

c. Application of the Two Percent Rule to Polymers Made from Telogens

If a telogen (i.e., a chain transfer agent) is used at greater than two percent by weight in the manufacture of a polymer, then this reactant is also part of the chemical name. In addition, for polymer names including the telogens, the term "telomer with" replaces the term "polymer with." If a telogen is used at less than or equal to two percent by weight and the manufacturer does not wish to include the telogen as part of the polymer identity, the substance is named using the term "polymer with" and the name of the telogen is omitted.

Example 45. 2-Propenoic acid, telomer with 1-dodecanethiol and 2-propenenitrile
CASRN 63747-59-1
C12H26S.(C3H4O2.C3H3N)x

Example 46. 2-Propenoic acid, telomer with 1-octanethiol, methyl 2-propenoate and sodium ethenesulfonate, ammonium salt
CASRN 70615-23-5
C8H18S.(C4H6O2.C3H4O2.C2H4O3S.Na)x.xH3N

d. Application of the Two Percent Rule to Cross-Linked Polymers and Prepolymers

As with any monomer or other reactant, if a cross-linking agent is used at greater than two percent by weight, the agent must be included in the polymer name. If a cross-linking agent is used at two percent or less by weight, the substance would be named without the chain-linking agent unless the submitter expresses a desire to include it.

For polymers manufactured from prepolymers, each of the ultimate monomers is subject to the two percent rule. If, for example, monomer E of prepolymer D-E is always present at less than or equal to two weight percent in the polymer A-B-C-D-E formed from prepolymer D-E, the resultant polymer incorporating monomers A, B, C and prepolymer D-E would be covered by the Inventory listing for polymer A-B-C-D. Manufacturers of polymers

that are made from prepolymers should remember that any prepolymer must itself be listed on the Inventory if it is to be used at any level in the domestic manufacture of another polymer. Thus, prepolymer D-E would have to be listed on the Inventory as such, even if monomer E were not part of the name of the final polymer.

2. Representation of Prepolymers

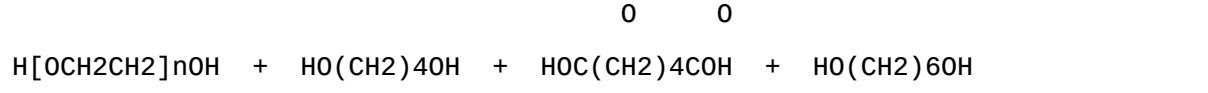
If a prepolymer is used in the manufacture of the polymer, it is usually listed in the description of the final polymer in terms of the monomers (and other reactants) used in its manufacture. Polymer nomenclature, including prepolymers, incorporates the identity of monomers and reactants used in the manufacture of the polymer. EPA treats component monomers (or other reactants) of any prepolymer as individual monomers/reactants as long as the prepolymer itself is identified just by monomer-based nomenclature. If this is the case and monomers A, B, C and prepolymer D-E are used to make polymer A-B-C-D-E, the polymer name would include the monomers A, B, C, D and E without reference to the prepolymer origin of D and E. For TSCA purposes, this polymer would be equivalent to one that was manufactured from the individual monomers, without first producing the prepolymer.

Example 47. If the prepolymer of 1,6-hexanediol and isophthalic acid is polymerized with caprolactone and dicyclohexylmethane 4,4'-diisocyanate, the resulting polymer is named according to ultimate monomers:

1,3-Benzenedicarboxylic acid, polymer with 1,6-hexanediol, 1,1'-methylenebis[4-isocyanatocyclohexane] and 2-oxepanone
CASRN 67599-34-2

Exception: If one or more monomers is described for TSCA purposes by an SRU name, its SRU identity will be maintained in the final polymer name.

Example 48.



CASRNs
25322-68-3 110-63-4 124-04-9 629-11-8

Hexanedioic acid, polymer with 1,4-butanediol, 1,6-hexanediol and .alpha.-hydro-.omega.-hydroxypoly(oxy-1,2-ethanediyl)
CASRN 71106-53-1

3. Structural Order or Arrangement of Monomers

Polymers on the Inventory are not distinguished by the structural order or arrangement of monomers (i.e., graft, block, alternating, and random), even though Chemical Abstracts Service assigns unique CAS Registry Numbers to these four different forms of the same polymeric substance.

For purposes of TSCA, EPA does not distinguish among these four forms, since the Agency does not distinguish among the ways in which the monomers line up structurally in the polymer, as long as the starting monomers and reactants do not change. The two polymers in the following example are considered to be identical for TSCA purposes.

Example 49. 2,5-Furandione, polymer with ethoxyethene
CASRN 26711-22-8

and

2,5-Furandione, polymer with ethoxyethene, alternating
CASRN 106209-34-1

The Agency uses the specific name attributed to the form of the polymer that is first added to the Inventory. If one of these four possible structural forms of a polymer is on the Inventory, the other forms are considered to be automatically on the Inventory as long as the starting monomers and reactants remain the same. The Agency does not add the names and CASRNs of any of these other polymer forms to the Inventory after the first reported form is commenced. Persons searching the Inventory should be aware of the various forms that a particular set of monomers could take and conduct their search accordingly.